

Carrier Localization, Metal-Insulator Transitions and Stripe Formation in Inhomogeneous Hole-Doped Cuprates

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We propose a unified approach for describing the carrier localization, metal-insulator transitions (MITs) and stripe formation in inhomogeneous hole-doped cuprates. The ground-state energy of a carrier interacting with a defect and with lattice vibrations is calculated variationally within the continuum model and adiabatic approximation. At low doping levels, hole carriers in La-based systems with large-radius dopants are localized near the dopants with the formation of hydrogen-like impurity centers. As the doping increases, the carriers are liberated from the hydrogen-like impurity centers and are self-trapped in a defect-free deformable lattice with the formation of intrinsic large polarons. In La-based cuprates with small-radius dopants, hole carriers are self-trapped near the dopants with the formation of non-hydrogen-like impurity centers or extrinsic large polarons. The charge ordering and formation of different superlattices and energy bands of dopants and intrinsic large polarons at their inhomogeneous spatial distribution trigger the MITs in cuprates. We analyse the validity of the criteria for the Mott and Anderson MITs in La-based cuprates with hydrogen-like impurity centers and show that such MITs in these systems are unlikely possible. Using the uncertainty principle we derive the quantitative criteria for the new MITs caused by strong carrier-dopant-phonon and carrier-phonon interactions. We show that the MITs in La-based cuprates with large-radius dopants are driven by intrinsic self-trapping and charge ordering, while the anisotropy of dielectric constants fosters the MITs accompanied by the formation of static stripes (in carrier-poor domains) and dynamic ones (in carrier-rich domains) in the range of doping $x \simeq 0.04-0.125$. The so-called $1/8$ anomaly is especially pronounced in these systems. The small-radius dopants and the anisotropy of dielectric constants favor carrier localization, MITs and stripe formation in a wide range of doping (including also "magic" doping $x=1/8$) in other La-based cuprates, where $x=1/8$ is no longer "magic" doping. Finally, the MIT and $1/8$ anomaly in cuprates caused by the commensurate ordering of planar large bipolarons and their condensation into a liquid are also discussed. The obtained results are in quantitative agreement with the experimental data on polaron formation, MITs and stripe formation in La-based cuprates.

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I. INTRODUCTION

The carrier localization, metal-insulator transitions (MITs) and stripe formation in hole-doped cuprates are the most challenging problems in condensed matter physics. These phenomena have attracted much attention because they are closely related to high- T_c superconductivity in cuprates¹⁻¹⁵. The mechanisms for carrier localization and MITs in the cuprates and related materials have been under discussion since the discovery of high- T_c superconductivity^{1-10,12,15,17-19}. Another important problem of the physics of high- T_c cuprates is the role of the electronic inhomogeneity and charge ordering in the stripe formation^{11,14,20,21}, which is intimately related to carrier localization and MITs in these materials. For cuprates within the insulating antiferromagnetic (AF) phase, the electron correlation is likely to dominate the carrier localization; when a MIT is approached, it is not obvious which process will dominate^{12,22}. Actually, the MITs in the cuprates might be different from the Mott and Anderson transitions. In these systems, the phenomena of carrier localization seem to be much more complicated by electron-defect-lattice and/or electron-lattice interaction effects which become very pronounced close to the MIT^{9,22}. Generally, the electron-defect-lattice

and/or electron-lattice interactions and the electronic inhomogeneity are known to foster carrier localization in solids. In particular, the strong electron-defect-phonon and electron-phonon interactions foster carrier localization by causing extrinsic and intrinsic self-trapping. At the same time the gross electronic inhomogeneities might play an important role in carrier localization, MITs and formation of insulating and metallic stripes in the cuprates. There is now increasing experimental evidence for the existence of extrinsic polarons (i.e., charge carriers self-trapped near the dopants or impurities), intrinsic polarons (or charge carriers self-trapped in a defect-free deformable lattice) and electronic inhomogeneities in these materials^{9,20,21,23,24}. In addition, various experiments on hole-doped La-based cuprates show that the MITs and stripe formation occur in underdoped (at doping levels $x = 0.05 - 0.125$)^{25,26}, optimally doped ($x = 0.15 - 0.16$)⁸, and overdoped ($x = 0.16 - 0.25$)^{16,21,27} regimes. However, the role of electronic inhomogeneities and strong carrier-defect-phonon and carrier-phonon interactions, which is known to be very important in the vicinity of the MITs^{20,22,28}, has not been fully explored in the underdoped regime. While the effects of ionic (or dopant) size and anisotropy of dielectric constants, which may play a key role in carrier localization and MITs,

have not been studied theoretically in inhomogeneous La-based cuprates in a wide hole concentration range from $x \sim 0.02$ (lightly doped regime) to $x \sim 0.25$ (heavily overdoped regime). In this work we examine such inhomogeneous systems in which the electronic charge inhomogeneities in conjunction with the strong carrier-defect-phonon and/or carrier-phonon interactions induce the carrier localization and MITs accompanied by the stripe formation in a wide range of doping. In so doing, we study the MITs and stripe formation in high- T_c cuprates driven by the inhomogeneous local doping, charge ordering and self-trapping of hole-carriers near defects (impurities) or in a defect-free deformable lattice.

This paper is organized as follows. First, in Sec. II, we investigate the extrinsic (or defect-assisted) and intrinsic self-trapping of carriers, and analyze the possibility of formation of extrinsic (hydrogen-like and non-hydrogen-like) and intrinsic self-trapped states in hole-doped La-based cuprates. Then, in Sec. III, we consider the possible forms of charge ordering and the formation of different superlattices and energy bands of dopants (i.e., acceptors) and intrinsic large polarons at their inhomogeneous spatial distribution. In Sec. IV, we examine the validity of the criteria for the Mott and Anderson transitions in La-based cuprates with hydrogenic impurity centers. We argue that such transitions in the cuprates are unlikely possible. We give our view of the new MITs in La-based cuprates with extrinsic large polarons (non-hydrogen-like impurity centers) or intrinsic large polarons and derive the quantitative criteria for the MITs by using the pertinent uncertainty relation. We show that in these systems the extrinsic and/or intrinsic self-trapping of hole carriers and the distinctly different charge ordering result in the new MITs which occur at different doping levels. Further, we find that, the ionic radius of dopants and the anisotropy of dielectric constants strongly influence on carrier localization, MITs, stripe formation and so-called 1/8 anomaly in La-based cuprates. These predictions are consistent with distinctive features of MITs, stripe formation and 1/8 anomaly observed in the cuprates. Finally, we briefly discuss the other type of MIT and the 1/8 anomaly in hole-doped cuprates caused by the commensurate ordering of planar large bipolarons and their condensation into a liquid. The paper concludes with Sec. V, in which the principle results are summarized.

II. EXTRINSIC AND INTRINSIC SELF-TRAPPING OF HOLE CARRIERS

The undoped layered cuprates are typical charge-transfer (CT)-type Mott insulators. According to the band calculations and spectroscopic data^{10,29}, the electronic structure of these parent CuO_2 -based compounds is well described by the three-band Hubbard model and the oxygen valence band lies within the Mott-Hubbard gap. Upon hole doping, the oxygen valence band of the cuprates is occupied by free holes. The hole carriers are

assumed to be within both a three-dimensional (3D) and two-dimensional (2D) deformable medium, the last one being CuO_2 layers^{1,6}. The large static dielectric constant ϵ_0 ($>> 10$) both parallel and perpendicular to the CuO_2 layers^{1,9} indicate that lattice ions may be significantly displaced in all three directions. In reality, the CuO_2 based materials may be approximated as a 3D deformable medium¹. As it was pointed out in Ref.³⁰, the existence of the 3D bismuth oxide high- T_c superconductors, which belong to the same class of materials as the copper oxides, casts an extra doubt on the theories based mainly on the low dimensionality of the crystal structure. There is also convincing experimental evidence that the consideration of cuprates as 3D systems may appear to be more appropriate (see Ref.^{12,31}). In these anisotropic 3D polar materials, the hole carriers interacting both with lattice vibrations (i.e., acoustic and optical phonons) and with lattice defects (e.g., dopants or impurities), can easily be self-trapped near the lattice defects. Such extrinsic self-trapping of hole carriers leads to the formation of a moderately deep extrinsic polaronic or a shallow hydrogenic state in the CT gap of the parent cuprates. The theory of carrier self-trapping has been developed in Refs.^{1,5,6,32,33} in the framework of the continuum approach. As shown in Refs.^{33,34}, the continuum theory of carrier self-trapping in a defect-free system can be easily extended to the system consisting of a defect and a bound charge carrier. Such a continuum approach is better suited for the quantitative analysis. In the framework of the continuum model, we make an attempt to analyze the possibility of the formation of hydrogen-like and non-hydrogen-like impurity states as well as polaronic ones in the CT gap of the cuprates.

The ground-state energy of a hole carrier in 3D polar crystals can be calculated variationally in the continuum model and adiabatic approximation, taking into account the short- and long-range carrier-defect-phonon interactions. The total energy of the interacting carrier-defect-phonon system is given by the functional³⁴

$$E\{\psi(r)\} = -\frac{\hbar^2}{2m^*} \int \psi(r) \nabla^2 \psi(r) d^3r - \frac{e^2}{2\tilde{\epsilon}} \int \frac{\psi^2(r)\psi^2(r')}{|r-r'|} d^3r d^3r' - \frac{E_d^2}{2K} \int \psi^4(r) d^3r - \frac{Ze^2}{\epsilon_0} \int \frac{\psi^2(r)}{r} d^3r + \left(V_0 - \frac{E_d E_{dD}}{K} \right) \int \psi^2(r) \delta(r) d^3r, \quad (1)$$

where $\psi(r)$ and m^* are the wave function and effective mass of a carrier, $\tilde{\epsilon} = \epsilon_\infty/(1-\eta)$ is the effective dielectric constant, $\eta = \epsilon_\infty/\epsilon_0$, ϵ_∞ is the high frequency dielectric constant, K is an elastic constant, E_d and E_{dD} are the deformation potentials of the carrier and the defect, respectively, V_0 is the short-range defect potential, Z is the charge state of the defect.

Now, we may choose the trial wave function $\psi(r)$ in

the Gaussian form

$$\psi(r) = N \exp [-(\sigma r)^2] \quad (2)$$

and make a variational calculation of Eq. (1) with respect to the parameters contained in $\psi(r)$, where $N = (2/\pi)^{3/4} \sigma^{3/2}$ is the normalization factor, $\sigma = \sqrt{\pi} \beta / a_0$ is the variational parameter, $\beta = a_0/a$ is the localization parameter, a is the radius of localization limited between a_0 (the lattice constant) and ∞ (free carrier). Inserting Eq. (2) into Eq. (1) and performing the r integration in Eq. (1), one can obtain the following functional

$$E(\beta) = B[\beta^2 - g_1 \beta^3 - g_2 \beta], \quad (3)$$

where $B = 3\pi \hbar^2 / 2m^* a_0^2$, $g_1 = (E_d^2 / 2K a_0^3 B)(1 + b_s)$, $b_s = 2^{5/2} [E_{dD} / E_d - KV_0 / E_d^2]$, $g_2 = (e^2 / \varepsilon_\infty a_0 B)(1 - \eta + b_l \eta)$, $b_l = 2^{3/2} Z$.

When $3g_1 g_2 < 1$ the functional (3) has a minimum at $\beta_{min} = [1 - \sqrt{1 - 3g_1 g_2}] / 3g_1$ which corresponds to the formation of a large-radius impurity state or extrinsic polaronic state in the CT gap of the doped cuprates. A carrier interacting with lattice vibrations becomes a large polaron with a polarization (or deformation) cloud extending over a wide region. We can determine the ground-state energy of such an intrinsic large polaron from Eq.(3) at $b_s=0$ and $Z=0$. At $3g_1 g_2 < 1$ the potential barrier height separating large- and small-radius self-trapped states of a hole carrier is equal to^{34,35}

$$E_a = \frac{4B}{27g_1^2} [1 - 3g_1 g_2]^{3/2}. \quad (4)$$

While the ground-state energy of a self-trapped carrier is given by³⁶

$$E(\beta_{min}) = \frac{B}{27g_1^2} \left[2 - 9g_1 g_2 - 2(1 - 3g_1 g_2)^{3/2} \right] \quad (5)$$

The signs of E_d and E_{dD} for holes and small-radius defects always positive, while E_{dD} for large-radius defects is negative³⁴. In $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) the radius of Sr^{2+} ions is larger than that of La^{3+} ions³⁷, so that for Sr^{2+} ion $Z=1$, $E_{dD} < 0$ and $b_s < 0$. In this case, the short-range part of the impurity potential in Eq. (1) is repulsive and the hole-lattice interactions near such dopants are suppressed by this repulsive defect potential. At a weak carrier-lattice interaction the localized impurity state may have hydrogen-like character described by a rigid lattice model³⁸. Therefore, in order to study the Mott MIT in LSCO, we can consider the hydrogenic impurity centers having the Bohr radius $a_H = 0.529 \varepsilon_0 (m_e / m^*) \text{\AA}$ and the ionization energy $E_I = e^2 / 2\varepsilon_0 a_H$ in the Hubbard model, where m_e is the free electron mass. However, the substitution of small-radius cations (e.g., Ca^{2+} and Nd^{3+} ions) for La^{3+} ions in La_2CuO_4 and for Sr^{2+} ions in LSCO leads to the formation of the non-hydrogenic impurity centers or extrinsic large polarons for which the Hubbard model is already inapplicable. The distinctive feature of the cuprates is

their very large ratio of static to high frequency dielectric constants^{1,39}. This situation is favorable for carriers attracted to polarization well created by the other ones or to Coulomb centers (dopants) to form 3D intrinsic or extrinsic large bipolarons. Such bipolarons with small binding energies can be formed in the lightly doped cuprates at $\eta < 0.1$ ³⁶ and they become unstable in the underdoped regime.

III. POSSIBLE TYPES OF CHARGE ORDERING AND FORMATION OF DIFFERENT SUPERLATTICES

The hole-doped cuprates are inhomogeneous or disordered systems, where the dopants and charge carriers are distributed inhomogeneously. Such dopant-driven and carrier-driven inhomogeneities may produce regions with different doping levels. The electronic inhomogeneity commonly exists in high- T_c cuprates regardless of doping level and the underdoped cuprates become more inhomogeneous than overdoped ones²⁰. Inhomogeneous distributions of carriers result from their interaction with one another (e.g. phase separation) and/or from their interaction with an inhomogeneous distribution of dopants or micro-structural defects such as dislocations³⁹. One can assume that the electronic disorder or inhomogeneity in the cuprates leads to the charge segregation into carrier-rich and carrier-poor regions. As the doping level increases towards underdoped region, specific charge ordering takes place in these regions and distinctly different superlattices and energy bands of dopants (impurities with trapped free carriers or large polarons) and self-trapped carriers (intrinsic large polarons) are formed at their inhomogeneous spatial distribution. In particular, the hydrogenic impurity centers (impurities with loosely bound free carriers or large polarons) and non-hydrogenic ones (impurities with tightly bound large polarons) are assumed to form the superlattices with the lattice constant a_I and coordination number z . The charge ordering in carrier-poor and carrier-rich domains results in the formation of simple cubic, body-centered cubic and face-centered cubic superlattices with coordination numbers $z=6, 8$ and 12 , respectively. In this case the formation of different impurity bands in the cuprates is described by the tight-binding approximation and the widths of the impurity bands can be determined from the relation

$$W_I = 2zJ_I, \quad (6)$$

where $J_I = \hbar^2 / 2m_I^* a_I^2$ is the hopping integral between nearest-neighbour impurity centers, m_I^* is the effective mass of charge carriers in the impurity band.

Further, we believe that the intrinsic large polarons just like impurity centers form different superlattices with the lattice constant a_p and the widths of the polaronic bands just as the widths of the small-polaron bands⁴⁰ are determined from the expression

$$W_p = 2zJ_p, \quad (7)$$

where $J_p = \hbar^2/2m_p^*a_p^2$ is the hopping integral between nearest-neighbour sites of the polaronic superlattice, m_p^* is the effective mass of large polarons.

At low doping level the extrinsic (or intrinsic) large polarons form a simple cubic superlattice with a_I or $a_p > 2R_p$, where R_p is the radius of the polaron. The width of the impurity band decreases with increasing inter-dopant separation, so that the impurity-band effective mass m_I increases with inter-dopant separation or with decreasing doping level. Clearly, in the lightly doped regime the narrow impurity and/or polaronic bands are formed in the CT gap of the parent cuprates and the energy gaps exist between the oxygen valence band and the impurity or polaronic bands. These energy gaps (or pseudogaps) disappear in sequence when the polaronic effects disappear in carrier-rich and carrier-poor domains in the overdoped regime.

We now make some remarks about the confinement energy of a large polaron and the width of the large-polaron band in the cuprates. The large-polaron confinement energy is about $\hbar^2/m_p R_p^{239,41}$. When the Fröhlich electron-phonon coupling constant α is large ($\alpha \gg 1$) the effective mass of a large polaron is given by the formula⁴⁰

$$m_p = \frac{16m^*}{81\pi^4}\alpha^4 \quad (8)$$

The Fröhlich coupling constant α for LSCO is estimated to be $\alpha = 5.7^{39,42}$. For $m^* = m_e^9$, we then obtain from (8), $m_p \simeq 2.14m_e$, which is close to the measured value of $m_p = 2m_e$ in LSCO⁹. Using the Bohr radius of the polaron $R_p = 0.529\varepsilon_0(m_e/m_p)\text{\AA} \simeq 7.42\text{\AA}$ (at $\varepsilon_0 = 30$) we obtain $\hbar^2/m_p R_p^2 \simeq 0.065\text{eV}$, which is less than E_p (see Sec. IV) and is larger than the characteristic phonon energies $\hbar\omega = 0.04\text{--}0.06\text{eV}$ in the cuprates^{9,23,43}. As the doping level is increased to underdoped levels at which the insulator-to-metal transition takes place, the distance between large polarons decreases and they can form closely packed simple cubic superlattice with $a_p = 2R_p$. In this case the large-polaron bandwidth is about $W_p \simeq 0.1\text{eV}$ (i.e., $W_p \gtrsim E_p$). In contrast, the small-polaron band will be very narrow ($W_p \ll \hbar\omega$) since the effective mass of a small polaron is much larger than a free-electron mass.

IV. METAL-INSULATOR TRANSITIONS AND STRIPE FORMATION

Now, we discuss how the extrinsic and/or intrinsic self-trapping of carriers, the dopant- and carrier-driven charge inhomogeneities and the charge ordering are related to the MITs and stripe formation in hole-doped cuprates. Various experiments have confirmed that for light doping, La_2CuO_4 behaves like a conventional semiconductor⁹. As described above, large-radius dopants or impurities with $E_{dD} < 0$ and $b_s < 0$ may form the hydrogenic acceptor centers in La-based cuprates and the Hubbard model based on the strong on-center

Coulomb repulsion U is applicable for studying the MIT in these systems. Then, the Mott MIT point is determined from the condition $W_I = E_I = 1.16U$ which was used in the derivation of the following criteria for the Mott MITs¹⁹: $n_c^{1/3}a_H \simeq 0.289$ ($z = 6$), $n_c^{1/3}a_H \simeq 0.315$ ($z = 8$) and $n_c^{1/3}a_H \simeq 0.324$ ($z = 12$), where n_c is the critical concentration of the hydrogenic impurities initiating the Mott MIT in doped systems. If we take $m^* = m_e$ (for free carriers) and $\varepsilon_0 = 30$, we find $a_H = 15.87\text{\AA}$ in LSCO. According to the above Mott criteria, the MITs would occur at the dimensionless hole concentrations $x_c = n_c/n_a \simeq 0.00115\text{--}0.00161$, where $n_a = 1/V_a$ is the density of the host lattice atoms, $V_a \simeq 190\text{\AA}^3$ is the volume per CuO_2 unit in the orthorhombic LSCO. The above values of x_c are much smaller than the value of $x_c \simeq 0.02$ at which the destruction of the antiferromagnetic (AF) order is observed in LSCO⁹. However, the large-radius dopant and large polaron may form the hydrogenic impurity center in LSCO. When $b_s < 0$ (or $E_{dD} < 0$), the defect and the self-trapped hole repel each other at short distance but attract each other at long distance. Therefore, the hydrogenic self-trapped state of a large polaron in LSCO has an effective Bohr radius $a_H = 0.529\varepsilon_0(m_e/m_p)\text{\AA}$. The existence of such hydrogenic acceptor centers in La-based cuprates is now experimentally well established⁹.

According to Mott and Davis³⁸, the Mott's criterion for the MIT can be used as the condition for the metallic behavior of a degenerate polaron gas if the Bohr radius a_H of polarons is larger than the interatomic distance. If we take $m_p = 2m_e$ and $\varepsilon_0 = 27$, we find $a_H \simeq 7.14\text{\AA}$, so that the above Mott criteria for the MITs can be applied to the cuprates. In this case the Mott transitions would occur at $x_c \simeq 0.0112\text{--}0.0178$. The quantitative criteria for the Anderson MITs, $n_c^{1/3}a_H \simeq 0.289$ (for $z=6$), $n_c^{1/3}a_H \simeq 0.293$ (for $z=8$), and $n_c^{1/3}a_H \simeq 0.272$ (for $z=12$), derived in Ref.¹⁹ predict nearly the same values of x_c . We see that the Mott transition (for shallow impurity centers) would occur at a much smaller dopant concentration than the critical doping concentration for the MIT in the cuprates. For example, the MITs in LSCO are observed at more higher doping levels $x_c \simeq 0.05\text{--}0.07^{2,3,10,16,25}$ and these experimental results cannot be reconciled with the above criteria for the Mott MITs. In our opinion, the hole carriers liberated from the large-radius dopants or hydrogenic impurity centers at $x_c \gtrsim 0.02$ are constrained to remain away from these impurities and they are self-trapped in a defect-free deformable lattice with the formation of strong-coupling intrinsic large polarons, which can acquire itineracy at higher doping levels²⁸.

Another possibility is that small-radius dopants (e.g., Ca^{2+} and Nd^{3+}) with $E_{dD} > 0$ (or $b_s > 0$) favor the formation of the extrinsic large polarons (non-hydrogenic impurity centers) in La-based cuprates. In the present case, both the short and long range parts of the carrier-defect interaction is attractive, so that hole carriers are

self-trapped near such dopants. Polaronic effects will be stronger near the small-radius dopants, leading to carrier localization over a broader range of doping. We can evaluate the possibility for the existence of a potential barrier separating large- and small-radius intrinsic polaronic states in 3D hole-doped La-based cuprates using the relation (4).

According to the spectroscopic data, the Fermi energy of the undoped cuprates is about $E_F \simeq 7\text{eV}^{44,45}$. To determine the value of the short-range carrier-phonon coupling constant g_1 , we estimate E_d as $E_d = (2/3)E_F$. The values of other parameters are $K = 1.4 \cdot 10^{12} \text{dyn/cm}^{246}$, $m^* = m_e^9$, $\varepsilon_\infty = 3 - 5^1$, $a_0 \simeq 6\text{\AA}$ (for orthorhombic LSCO), $b_s = 0$ and $Z = 0$. Then $B = 1\text{ eV}$, $g_1 \simeq 0.0576$ and $g_2 \simeq 2.4(1 - \eta)/\varepsilon_\infty$. For the cuprates, typical values of η range from 0.02 to 0.12⁹. Using Eq.(4), we obtain E_a value of $\sim 38\text{ eV}$ at $\varepsilon_\infty = 4$ and $\eta = 0.06$. As already seen, the large- and small-radius polaronic states are separated by very high potential barrier. This barrier prevents the formation of small polarons in the 3D cuprates. At $b_s = 0.5$ and $Z = 1$ the height of such a potential barrier separating large- and small-radius extrinsic polaronic states is $\sim 14\text{ eV}$. It follows that the relevant charge carriers in the anisotropic 3D cuprates are the large intrinsic and extrinsic polarons (or bipolarons). While the small polarons and bipolarons may be formed in the CuO_2 layers of the cuprates, where the self-trapping of carriers may occur more easily due to the absence of the potential barrier between the large- and small-radius self-trapped states in 2D systems^{47,48}. However, such (bi)polarons having very large effective masses and narrow energy bands tend to be localized rather than mobile.

Small or large polarons may be expected in polar materials with a small or large hopping integral J between nearest-neighbour sites of the crystal lattice. The radius of the polaron R_p is of order $a_0(2J/E_p)$ and the formation of a polaron whose radius is large compared to the lattice constant a_0 requires that $2J/E_p \gg 1$ (see also Ref.⁴⁹) or $W_p/E_p > 1^{50}$. In hole-doped cuprates (LSCO, $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$) large polarons have the effective masses $m_p \simeq (2 \div 4)m_e^{9,51}$. Therefore, W_I and W_p may be comparable with the binding energies E_p^I and E_p of the extrinsic and intrinsic large polarons since $m_p, m_I (\gtrsim m_p)$, a_I and a_p would decrease with increasing carrier concentration. At $m_I \lesssim 2m_e$ and $m_p \lesssim 2m_e$ the magnitudes of W_I and W_p may become larger than E_p^I and E_p , which are determined from Eq.(5) by using the above presented values of parameters. The obtained results are summarized in Table 1. When η increases, the ionization energy E_p^I of the non-hydrogenic impurity centers (with $Z = 1$) increases. On the contrary, the binding energy of the intrinsic large polarons E_p decreases. Interestingly, E_p^I and E_p increases markedly with decreasing ε_∞ from 5 to 3. We see that the value of $E_p^I = 0.13\text{ eV}$ obtained at $\eta = 0.10$ and $Z = 1$ is consistent with the experimental data for lightly doped $\text{La}_2\text{CuO}_{4+y}$ ⁹ and the impurity band observed in these

TABLE I: Binding energies of intrinsic and extrinsic large polarons for $\varepsilon_\infty = 4$, $b_s = 0.5$ and different values of η .

η	0.00	0.02	0.04	0.06	0.08	0.10	0.12
E_p, eV	0.0916	0.0879	0.0844	0.0809	0.0774	0.0741	0.0708
$Z = 0$							
E_p^I, eV	0.0925	0.0888	0.0851	0.0816	0.0781	0.0747	0.0714
$Z = 1$							
E_p^I, eV	0.0925	0.0995	0.1067	0.1142	0.1220	0.1301	0.1384

systems at 0.13 eV is associated with the extrinsic large polarons rather than the small polarons bound to impurities.

As we have discussed above, the extrinsic large polarons bound to dopants may also form different superlattices in inhomogeneous hole-doped cuprates and the energy bands (which are formed in the lightly doped cuprates) of such polarons may exist, thus permitting charge transport by means of intra-band conduction. In case of narrow polaronic bands, charge transport becomes hopping-like and is caused by intra-band hopping processes⁵². One can assume that if the bandwidth of the extrinsic large polarons exceeds some critical value, their intra-band conduction becomes metal-like. We attempt to find the new criteria for such MITs in doped materials.

When the carrier concentration is low, the carriers occupy low-lying bound states (i.e., extrinsic or intrinsic polaronic states) first. As soon as all the localized states were filled at some critical carrier concentration $n = n_c$ (or $x = x_c$), the carriers start to occupy the itinerant states and the transition of the system from the insulating phase to the metallic one occurs. The possible values of n_c at which extrinsic or intrinsic large polarons forming different superlattices acquire itineracy are determined from the appropriate criteria for the MITs. The conditions for carrier localization or delocalization can be obtained by using the uncertainty principle: $\Delta p \Delta x \geq \hbar/2$, where Δp and Δx are the uncertainties in the momentum and coordinate, respectively. This uncertainty relation can be written as

$$\Delta x \cdot \Delta E \simeq \frac{\hbar^2(\Delta k)^2}{2m^*} \cdot \frac{1}{2\Delta k}, \quad (9)$$

where ΔE and Δk are the uncertainties in the energy and wave vector, respectively. The expression $\hbar^2(\Delta k)^2/2m^*$ in Eq. (9) represents the uncertainty in the energy of free carriers. Taking into account that the uncertainties in the energy and wave vector in the impurity band are about W_I and $1/a_I$, respectively, the relation (9) can be rewritten in the form (cf. a similar relation formerly derived by Ridley⁴¹ using the uncertainty principle)

$$\Delta x \cdot \Delta E \cong W_I a_I / 2 \quad (10)$$

On the other hand, the uncertainty in the energy ΔE of the localized state of carriers is of the order of E_p^I ,

whereas the uncertainty in the coordinate Δx of the extrinsic large polarons is of the order of the polaron radius R_I . Then, the condition for the setting-in of carrier localization can be written as

$$E_p^I R_I \gtrsim W_I a_I / 2, \quad (11)$$

so that the new criterion for the MIT can be derived from this condition and written as

$$\frac{E_p^I}{W_I} = 0.5 \frac{a_I}{R_I}, \quad (12)$$

which is similar to the results for analogous problems of Holstein localization, Mott and Anderson MITs. In particular, localization in the one-dimensional Holstein molecular-crystal model is governed by the ratio of the local polaron binding energy to the inter-site bandwidth^{39,53}. Similarly, Anderson's localization in Anderson's disorder model is governed by the ratio of the local-site energy (or the random potential V_0) to the electron bandwidth and Mott's MIT is governed by the ratio of the Hubbard on-site Coulomb interaction energy U to the W ^{38,41,52}. For intrinsic large polarons, instead of (12), we could write

$$\frac{E_p}{W_p} = 0.5 \frac{a_p}{R_p}. \quad (13)$$

With increasing the inter-polaron distance R , the polaron band is continuously narrowed, finally ending in the discrete levels (at $R \gg R_p$) of the non-interacting polarons. On the contrary, with decreasing R , the large polarons begin to interact one another through the overlap of their structural distortions and the polaronic states are broadened into an energy band. As long as the distance between nearest-neighbour polarons is larger than $2R_p$ and the overlap of the deformation clouds of polarons is small, one would expect the large-polaron bands to be very narrow. In this case large polarons are localized or confined to their potential wells and the system is converted into an insulator. For $R = 2R_p$ (which is assumed to correspond to the packing of spheres with radii equal to the polaron radius), the deformation clouds of large polarons begin to overlap strongly and the large polarons are delocalized and characterized by metal-like transport in sufficiently broadened energy bands.

If the extrinsic large polarons form such closely packed simple cubic, body-centered cubic and face-centered cubic superlattices with $a_I = 2R_I$ ($z = 6$), $a_I = (4/\sqrt{3})R_I$ ($z = 8$) and $a_I = (2\sqrt{2})R_I$ ($z = 12$), the appropriate densities of such carriers per unit cells of the superlattices are $n = 1/a_I^3$, $n = 2/a_I^3$ and $n = 4/a_I^3$, respectively. For these cases, three successive MITs are feasible and the localized extrinsic large polarons in the cuprates start to occupy the itinerant states at different hole concentrations determined from relation (12). This means that the system gradually changes from the insulating phase to the metallic one. When the extrinsic large polarons form simple cubic and face-centered cubic superlattices,

such insulator-to-metal transitions occur at $W_I = E_p^I$ and $W_I = E_p^I/\sqrt{2}$, respectively. We argue that the electronic inhomogeneities and the ordering of polaronic carriers with the formation of different superlattices can produce various types of self-organized electronic structures in the form of stripes. Using the relation (12), we obtain the following criteria for the new MITs:

$$n_c = \left(\frac{m_I E_p^I}{z \hbar^2} \right)^{3/2} \quad \text{for } z = 6, \quad (14)$$

$$n_c = \frac{1}{\sqrt{2}} \left(\frac{\sqrt{3} m_I E_p^I}{z \hbar^2} \right)^{3/2} \quad \text{for } z = 8, \quad (15)$$

$$n_c = 2^{5/4} \left(\frac{2 m_I E_p^I}{z \hbar^2} \right)^{3/2} \quad \text{for } z = 12. \quad (16)$$

We are now in a position to evaluate n_c in La-based cuprates using Eqs. (14), (15) and (16). The effective masses of carriers in cuprates deduced from ARPES and electronic specific heat data (see Ref.⁵⁴) at different doping levels are slightly different and equal to 2.1 - 2.5 times the free electron mass. Therefore, we can evaluate n_c by taking $m_I = 2.5m_e$ for $\text{La}_{2-x}\text{Ca}_x\text{CuO}_4$. Then for $\eta = 0.02$ and $E_p^I = 0.10\text{eV}$ we find $x_c \simeq 0.065 - 0.080$. When $\varepsilon_\infty = 4$, $\eta = 0.02 - 0.12$ and $E_p^I = 0.100 - 0.138\text{eV}$ (see Table 1), the MITs and stripe formation occur in these systems at $x_c \simeq 0.065 - 0.131$. At $\varepsilon_\infty = 3$ and $\eta = 0.06$ we obtain $E_p^I \simeq 0.2\text{eV}$. Then the metal-insulator boundary of $\text{La}_{2-x}\text{Ca}_x\text{CuO}_4$ lies in the overdoped regime at $x_c \simeq 0.226$ (for $z = 8$).

Further, the double substitution of smaller cations for host lattice ions and dopants may also favor the MITs and stripe formation occurring in a wide range of doping of La-based cuprates. When the doping increases, there is a significant probability of at least two neighbouring La^{2+} ions replaced by large-radius Sr^{2+} ion (with $Z = 1$, $V_0^{Sr} > 0$ and $E_{dD}^{Sr} < 0$) and by small-radius Nd^{3+} ion (with $Z = 0$, $V_0^{Nd} > 0$ and $E_{dD}^{Nd} > 0$) in $\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4$ (where $y \gg x$). The attractive potentials of these two-dopant centers may be greater than those of more separated dopants. For $\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4$ with such two-dopant centers, we should replace V_0 and E_{dD} by $V_0^{Sr} + V_0^{Nd}$ and $E_{dD}^{Sr} + E_{dD}^{Nd}$ in Eq.(1) or in the expression for b_s . At $E_{dD}^{Sr} + E_{dD}^{Nd} > 0$ (i.e., $b_s > 0$) the short-range part of the two-dopant potential is attractive and the hole carriers are self-trapped near the two neighbouring dopants with the formation of the extrinsic large polarons. The two-dopant-driven charge inhomogeneity and ordering lead to formation of the superlattices of such extrinsic large polarons. In order to illustrate the effects of anisotropy of ε_∞ and the short-range defect potential on x_c , we show in Fig.1 results of our calculations

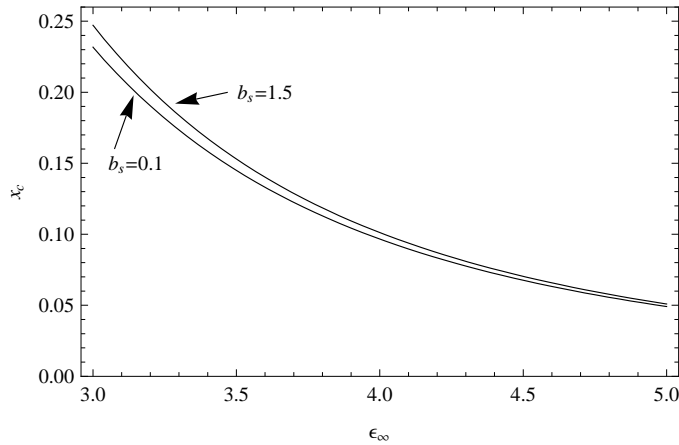


FIG. 1: Critical carrier concentration x_c as a function of ϵ_∞ at $z = 8$, $\eta = 0.06$, $b_s = 0.1$ and $b_s = 1.5$.

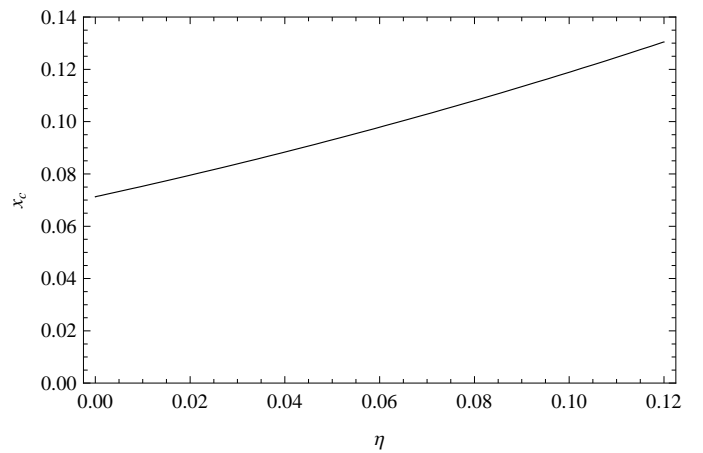


FIG. 2: Critical carrier concentration x_c as a function of η at $z = 8$, $b_s = 0.5$ and $\epsilon_\infty = 4$.

for hole-doped La-based cuprates with two-dopant centers for which $Z = 1$ and $b_s > 0$. Fig.1 shows that the anisotropy of ϵ_∞ and the size effect of small-radius dopants are the main driving forces for the new MITs and stripe formation in a wide range of doping (including also $x = 1/8$) in La-based cuprates containing two types of dopants (i.e., large- and small-radius dopants). Indeed, in hole-doped cuprates $\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4$ and $\text{La}_{2-x-y}\text{Eu}_y\text{Sr}_x\text{CuO}_4$ with small-radius dopants Nd^{3+} and Eu^{3+} , the static stripe phases are observed in a wide range of carrier concentration and not restricted to a narrow range around $x = 1/8$ in which superconductivity is suppressed^{16,27,55}.

As mentioned above, the size of impurities is also a key parameter in the cuprates containing large-radius dopants and the formation of intrinsic large polarons in these systems becomes possible at distances far from the impurities. Such materials are the compounds LSCO and $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ (LBCO) in which large polarons form different superlattices and acquire itineracy at some critical carrier concentrations n_c determined from the relations (14), (15) and (16) by replacing m_I and E_p^I by m_p and E_p in these relations. Using the values of $\eta = 0.02$, $\epsilon_\infty = 4$, $m_p = 2.1m_e$ and $E_p \simeq 0.088\text{eV}$ (see Table 1) for LSCO and LBCO, we find $x_c \simeq 0.049$ (for $z=6$) and $x_c \simeq 0.051$ (for $z=8$). These values of x_c are in excellent agreement with the experimental value $x_c = 0.05$ in LSCO¹⁰. If we take into account a possible anisotropy of $\epsilon_\infty = 3 - 4$ and $\eta = 0.02 - 0.10$, then we obtain $x_c \simeq 0.04 - 0.125$, which are also well consistent with existing experimental data on MITs and stripe formation in LSCO and LBCO (see Refs.^{10,22,26,55}). In Fig. 2 we plot the dependence of x_c on η for $z = 8$, $b_s = 0.5$ and $\epsilon_\infty = 4$. Fig.2 shows that the value of x_c increases markedly with increasing η for the cuprates containing large-radius dopants. Our results clearly indicate that $x = 1/8$ is truly "magic" or particular doping level for hole-doped cuprates LSCO and LBCO. In these systems, the suppression of superconductivity should be expected for x

close to $1/8$. However, the doping level $x = 1/8$ is not "magic" doping level for the formation of stripes in other hole-doped cuprates, where the effects of small-radius dopants on MITs and static stripe formation are strong enough. The stripe formation driven by the MITs occurs in such systems not only at $x = 1/8$ but also at much more higher doping levels. Indeed, experimental studies on $\text{La}_{2-x}\text{Ba}_{x-y}\text{M}_y\text{CuO}_4$ (where $M = \text{Sr}, \text{Ca}$) show that the $1/8$ anomaly is reduced by substituting smaller divalent cations instead of large-radius Ba^{2+} ⁵⁵. In contrast, the ordering of intrinsic large polarons is important for the MITs and stripe formation in LSCO and LBCO. Double doping experiments on $\text{La}_{2-x-y}\text{Ba}_x\text{Th}_y\text{CuO}_4$ indicate that superconductivity is suppressed when the hole concentration $p = x - y$ (not the individual or total dopant concentrations x , y and $x + y$) is $1/8$ ^{56,57}. In this system, the Th^{4+} ion acts to compensate the negative effective charge of Ba-site, so that the hole concentration is now given by $p = x - y$. This means that the presumed superlattice and stripe formation accompanied by the suppression of superconductivity in $\text{La}_{2-x-y}\text{Ba}_x\text{Th}_y\text{CuO}_4$ are associated with the ordering of intrinsic large polarons³⁹ rather than dopants.

The formation of 3D and 2D large bipolarons is also expected in the cuprates^{1,5,6,58-60}. Such bipolarons can only exist if the Fröhlich coupling constant α is greater than the critical value α_c and when η is smaller than the critical value η_c . For instance, for 3D and 2D systems, the following critical parameters were obtained by using the Gaussian type trial wave functions: $\alpha_c^{(3D)} \simeq 5.8$, $\eta_c^{(3D)} \simeq 0.13$ ^{6,59} and $\alpha_c^{(2D)} \simeq 2.94$, $\eta_c^{(2D)} \simeq 0.167$ (for $\alpha = 5$), $\eta_c^{(2D)} \simeq 0.173$ (for $\alpha = 10$)⁶⁰. The ratio of 3D bipolaron binding energy E_{bB} to twice the polaron energy $2E_p$ is about $E_{bB}/2E_p \simeq 0.22$ at $\eta \rightarrow 0$ ⁶¹, whereas the ratio of 3D extrinsic bipolaron binding energy E_{bB}^I to twice the extrinsic polaron energy $2E_p^I$ is somewhat smaller than the value of $E_{bB}/2E_p$ ⁶². Furthermore, the binding energies of 3D extrinsic and intrinsic large bipo-

larons decrease with the increase of η . Therefore, such bipolarons may exist at low doping levels. As the carrier concentration increases, 3D large bipolarons dissociate first into two large polarons and then these polarons acquire itineracy at a higher doping level $x = x_c$ which corresponds to the onset of the metallic behavior of the system. However, the properties of 2D large (bi)polarons may be quite different from those of 3D large (bi)polarons. It is clear that the binding energy and the effective mass of a bipolaron would increase greatly with decreasing dimensionality. In particular, the binding energy of 2D large bipolarons $E_{bB}^{(2D)}$ is expected to be much greater than $E_{bB}^{(3D)}$. The 2D polaron and bipolaron ground-state energies $E_p^{(2D)}$ and $E_{bB}^{(2D)}$ can be obtained approximately using the scaling relations^{58,63}:

$$E_p^{(2D)}(\alpha) = \frac{2}{3}E_p^{(3D)}((3\pi/4)\alpha) \quad (17)$$

and

$$E_B^{(2D)}(\alpha, U) = \frac{2}{3}E_B^{(3D)}\left(\frac{3\pi}{4}\alpha, \frac{3\pi}{4}U\right), \quad (18)$$

where $E_p^{(3D)}$ and $E_B^{(3D)}$ are the 3D polaron and bipolaron ground-state energies, respectively, U is the strength of the Coulomb repulsion between the pairing carriers.

In the strong coupling regime $\alpha > \alpha_c$, the ground-state energies of 3D large polaron and bipolaron are proportional to α^{259} . In this case the 2D large bipolaron binding energy is given by

$$E_{bB}^{(2D)} = \frac{2}{3}\left(\frac{3\pi}{4}\right)^2 E_{bB}^{(3D)} \simeq 3.7E_{bB}^{(3D)} \quad (19)$$

from which it follows that the bipolaron binding energy will be much larger in 2D systems as compared to 3D ones and, therefore, 2D bipolarons will be strongly localized. Such 2D large bipolarons will unlikely be dissociated in underdoped and optimally doped cuprates. According to Emin^{5,39,64,65}, quasi-2D large bipolarons are attracted to one another via the phonon-mediated interaction that fosters their condensation into a normal liquid. Carriers are assumed to condense into droplets and form a liquid prior to their condensing further into a superconducting state³⁹. The concentration of such large bipolarons above which they condense into a normal liquid at a reasonable temperature is assumed to be $x_{bi}^{crit} \sim 0.1/n_{bi}$ ^{5,39}, where n_{bi} is the number of unit cells involved in a large bipolaron. To form one bipolaron, two carriers are required from two dopants, then the critical doping level is $x_c = 2x_{bi}^{crit}$. Envisioning a large bipolaron involving about five cells, one cell and its four neighbors, the critical carrier concentration for forming a large-bipolaron liquid is about $x_c \simeq 0.2/5 = 0.04$ ^{5,39}. It was also suggested^{5,39} that in the cuprates, superconductivity occurs when the dopant density exceeds the density of a large bipolaron liquid, namely, at $x_c \gtrsim 0.05$, and large-bipolaron superconductivity of

the cuprates is determined by the competition between large-bipolarons' attraction for one another and their attraction to dopants. At the same time the condensation of attracting large bipolarons (including also Cooper pairs of large polarons) into a superfluid Bose-liquid in the cuprates below the superconducting transition temperature T_c was suggested in Refs.^{66,67}. The condensation of large bipolarons into a superfluid Bose-liquid at sufficiently low temperatures in the cuprates can be regarded as an insulator-to-superconductor transition²⁸. Emin argued^{5,39,64,65} that (bi)polarons in the cuprates order in a manner commensurate with the underlying lattice, thereby forming a superlattice. For the square structure of CuO_2 planes such a commensurate ordering of large bipolarons can occur at $x = 1/8$ and lead to the conversion of a cuprate superconductor to an insulator composed of ordered large bipolarons⁶⁸. Thus, the type of transition proposed by Emin is another possibility of the metal-to-insulator (at $T > T_c$) or superconductor-to-insulator (at $T \lesssim T_c$) transition which is driven by the commensurate ordering of quasi-2D large bipolarons and presumed superlattice formation. It is believed³⁹ that such transitions are neither a Mott transition nor an Anderson transition.

V. CONCLUSIONS

In this paper we have studied the carrier localization, MITs and stripe formation in inhomogeneous hole-doped cuprates driven by the gross electronic inhomogeneities, charge ordering and extrinsic and/or intrinsic self-trapping of hole carriers. To model the real situation in cuprates, the hole carriers are presumed to exist in a 3D ionic continuum medium and interact with the dopants (or impurities) via short and long-range carrier-defect-lattice interactions and with the lattice vibrations via short and long-range carrier-lattice interactions. We have investigated the self-trapping of carriers near the defects and away from the defects (i.e., in a defect-free deformable lattice) within the continuum model and adiabatic approximation. Then, the possibility of the formation of extrinsic self-trapped states (i.e., hydrogenic and non-hydrogenic acceptor states) and intrinsic ones (large-polaronic states) in the CT gap of the cuprates is examined. We think that the large-radius dopants with the short-range repulsive potential can form hydrogenic impurity centers in LSCO and LBCO, where the hole carriers liberated from such impurity centers are self-trapped in a defect-free deformable lattice due to the strong short and long-range carrier-lattice interactions. When such hydrogenic impurity centers are distributed inhomogeneously and ordered differently with the formation of distinctly different superlattices, the narrow Hubbard impurity bands are formed in the CT gap of the cuprates. We have analyzed the applicability of the newly derived criteria for the Mott and Anderson MITs to the La-based cuprates. It is found that such MITs in

the cuprates with the hydrogenic impurity centers are unlikely possible. The situation in La-based cuprates with small-radius dopants is quite different from LSCO and LBCO cases. In these systems, the short- and long-range parts of the small-radius dopant potential are attractive and the combined effect of the strong carrier-defect and carrier-lattice interactions fosters carrier localization (or defect-assisted self-trapping of carriers) and formation of extrinsic large polarons. We have calculated the ground state energies (i.e., binding energies) of extrinsic and intrinsic large polarons in La-based cuprates. The obtained results are consistent with experimental results on polaron formation in these systems.

Further, we have demonstrated that the driving forces for carrier localization, MITs and stripe formation in La-based cuprates are the extrinsic and/or intrinsic self-trapping of hole carriers, the dopant and carrier-driven electronic inhomogeneities, the charge ordering and the anisotropy of dielectric constants. Under the certain conditions, the narrow energy bands of extrinsic and intrinsic large polarons are assumed to prelude itinerant motion of such polarons. These conditions and quantitative criteria for the new MITs in inhomogeneous La-based cuprates are obtained by using the pertinent uncertainty relation. We showed that the new MITs are accompanied by the formation of static and dynamic stripes, and would occur at different critical carrier concentrations depending on the ionic size of dopants (or impurities), the anisotropy of dielectric constants and the type of the ordering of extrinsic and/or intrinsic large polarons. In particular, the ordering of 3D intrinsic large polarons, the formation of different polaronic superlattices ($z = 6$ and 8) and the anisotropy of dielectric constants favor the MITs and stripe formation in the range of doping $x = 0.04 - 0.125$ in La-based cuprates with large-radius dopants. We argue that the $x = 1/8$ anomaly is characteristic of these cuprates, where the suppression of superconductivity due to the formation of static stripes should be especially pronounced for the doping level $x = 1/8$. While the effects of the substitution of smaller cations for host lattice ions or dopants (e.g., Nd^{3+} in LSCO), the anisotropy of dielectric constants and the ordering of extrinsic large polarons with the formation of different superlattices ($z = 6$ and 8) extend the metal-insulator

crossover region from the heavily underdoped ($x = 0.04$) to the overdoped ($x > 0.2$) regime. Our results suggest that the new MITs and the formation of static stripes (in carrier-poor domains) and dynamic ones (in carrier-rich domains) occur in a wide range of doping (including also the "magic" doping $1/8$) in La-based cuprates containing small-radius dopants (e.g., Ca^{2+} and Nd^{3+} ions), where the hole concentration $x = 1/8$ is not already particular doping level corresponding to the formation of static stripes.

When 3D extrinsic and intrinsic large bipolarons are formed in the cuprates at $\eta < \eta_c$, such bipolarons will dissociate first into two large polarons at low carrier concentration and then these polarons become mobile or acquire itineracy at high doping levels $x \geq x_c \simeq 0.05$. The essence of the above driving forces for carrier localization, MITs and static stripe formation in La-based cuprates has been mimicked by the theoretical predictions which capture the main characteristics of experiment. Thus, we have succeeded in explaining the experimental results on carrier localization, MITs and stripe formation in hole-doped La-based cuprates with large- and small-radius dopants in the two characteristic doping regimes $0.05 \leq x \leq 0.125$ and $0.05 \leq x \leq 0.25$, respectively.

Finally, it should be noted that carrier localization and metal (or superconductor)-to-insulator transition accompanied by the $1/8$ anomaly in hole-doped cuprates might be also driven by the commensurate ordering of quasi-2D (or planar) large bipolarons which will condense into a liquid above some critical carrier concentration.

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Abstract

